

Many-body Green's function theory of ferromagnetic Heisenberg systems with single-ion anisotropies in more than one direction

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The behaviour of ferromagnetic systems with single-ion anisotropies and magnetic fields in more than one direction is investigated with many-body Green's function theory generalizing earlier work with uniaxial anisotropies only. It turns out to be of advantage to construct Green's functions in terms of the spin operators S^x, S^y and S^z , instead of the commonly used S^+, S^- and S^z operators. The exchange energy terms are decoupled by RPA and the single-ion anisotropy terms by a generalization of the Anderson-Callen decoupling. We stress that in the derivation of the formalism none of the three spatial axes is special, so that one is always able to select a reference direction along which a magnetization component is not zero. Analytical expressions are obtained for all three components of the magnetization and the expectation values $\langle (S^x)^2 \rangle$, $\langle (S^y)^2 \rangle$ and $\langle (S^z)^2 \rangle$ for any spin quantum number S . The formalism considers both in-plane and out-of-plane anisotropies. Numerical calculations illustrate the behaviour of the magnetization for 3-dimensional and 2-dimensional systems for various parameters. In the 2-dimensional (monolayer) case, the magnetic dipole-dipole coupling is included, and a comparison is made between in-plane and out-of-plane anisotropies.

I. INTRODUCTION

The spontaneous magnetization of bulk ferromagnets has been successfully described by a Heisenberg model within the framework of many-body Green's function theory^{1,2,3}, where the Tyablikov decoupling (random phase approximation: RPA) is the crucial approximation for the exchange energy term. Usually, only the z -component of the magnetization $\langle S^z \rangle$ was considered. Callen³ developed a formalism which lead to a closed-form expression for the magnetization $\langle S^z \rangle$ in ferromagnetic (FM) systems for any spin quantum number S . This theory has been helpful in studying various systems described by Heisenberg Hamiltonians^{4,5,6,7}.

Recently, experimental work has provided an incentive to calculate more than one component of the magnetization. For example, under the influence of an external field perpendicular to the anisotropy axis, the magnetization rotates with the variation of the field strength. When a FM layer is covered by an anti-ferromagnetic layer, the magnetizations across the interface may have different orientations⁸. Moreover, the antiferromagnetic sublattice magnetization may be non-collinear⁹. In FM ultrathin films, the magnetization may rotate when the temperature or film thickness are varied; see e.g.^{10,11,12,13}.

Fröbrich et al.^{12,13} have developed a method using Green's function theory to calculate more than one component of the magnetization for FM films. They investigated the reorientation of the magnetization of FM films caused by an external field and the dipole-dipole coupling by applying RPA to the exchange energy term and the Anderson-Callen decoupling¹⁴ to an *out-of-plane* single-ion anisotropy. Later an exact treatment of the single-ion anisotropy term was proposed by going to higher-order Green's functions¹⁵. This exact treatment and a comparison with Quantum Monte Carlo calculations¹⁶ showed that the Anderson-Callen decoupling is a good approximation when the single-ion anisotropy is small compared to the exchange interaction. The Anderson-Callen decoupling can therefore often be a useful approximation in this situation, particularly as it is much simpler to apply than the exact treatment. In Ref.¹⁷, general analytical formulas were derived on the basis of RPA and the Anderson-Callen decoupling for the three components of the magnetization for 3D and 2D FM systems for any spin quantum number. The Green's function formalism was also applied to uniaxial out-of-plane and uniaxial in-plane *exchange* anisotropies^{18,19,20}.

The papers above [12-17] dealt only with a uniaxial *out-of-plane* single-ion anisotropy. In the present paper, we generalize the model by introducing single-ion anisotropies in all directions of space, thus obtaining the in-plane and

out-of-plane anisotropies as special cases, and also allowing for a reorientation of the magnetization from out-of-plane to in-plane and vice versa, depending on the chosen parameters. The new key features are the formulation in terms of Green's functions defined in the spin operators S^x, S^y, S^z instead of the S^+, S^-, S^z operators, and the generalization of the Anderson-Callen decoupling to the terms coming from the single-ion anisotropies for all directions in space. The new formulation is advantageous if several non-vanishing components of the magnetization are present.

The paper is organized as follows. Section 2 presents the general formalism for any spin quantum number. Section 3 shows numerical results for the 3D case and for a monolayer film (2D). For the latter case we also discuss the effects of the magnetic dipole-dipole coupling. Section 4 contains our conclusions.

II. THE FORMALISM

The Hamiltonian for a ferromagnetic system is

$$H = -\frac{J}{2} \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_i [K_{2x}(S_i^x)^2 + K_{2y}(S_i^y)^2 + K_{2z}(S_i^z)^2] - \sum_i \mathbf{B} \cdot \mathbf{S}_i. \quad (1)$$

The first term is the Heisenberg exchange interaction ($J > 0$). The second term describes single-ion anisotropies in all three directions of space where we assume that the anisotropy constants are greater or equal to zero, $K_{2\alpha} \geq 0$ for $\alpha = x, y, z$. Note, that due to the exact relation $(S^x)^2 + (S^y)^2 + (S^z)^2 = S(S+1)$ only two of the $K_{2\alpha}$ are independent. The third term is the Zeeman energy, arising from an external magnetic field.

We use retarded many-body Green's functions defined in accordance with Bogolyubov and Tyablikov²¹ as

$$G_{ij,\eta}(t-t') = \langle \langle A_i; B_j \rangle \rangle_\eta = -i\theta(t-t') \langle [A_i, B_j]_\eta \rangle, \quad (2)$$

where the operators A_i and B_j depend on the problem under consideration, and the subscripts i and j label lattice sites. $\theta(t-t')$ is the Heaviside function, and $\langle \dots \rangle$ denotes the thermodynamical expectation value. Furthermore

$$[A_i, B_j]_\eta = A_i B_j + \eta B_j A_i = F_{ij,\eta}, \quad \eta = \pm 1. \quad (3)$$

After a Fourier transformation to energy space, we obtain the equation of motion:

$$\omega \langle \langle A_i; B_j \rangle \rangle_{\eta,\omega} = \langle [A_i, B_j]_\eta \rangle + \langle \langle [A_i, H]; B_j \rangle \rangle_{\eta,\omega}. \quad (4)$$

The Green's function is further Fourier transformed to momentum space

$$g(\mathbf{k}, \omega) = \frac{1}{N} \sum_{ij} G_{ij}(\omega) e^{i\mathbf{k} \cdot (\mathbf{i}-\mathbf{j})}. \quad (5)$$

The aim is to obtain the Green's function $g(\mathbf{k}, \omega)$ from a solution of the equations of motion. Then, statistical averages of the product of the two operators B_j and A_i (correlation functions), may be cast in terms of correlations in momentum space, $C_{\mathbf{k}}$:

$$\langle B_j A_i \rangle = \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot (\mathbf{i}-\mathbf{j})} C_{\mathbf{k}}. \quad (6)$$

The $C_{\mathbf{k}}$ can be calculated by the well-known spectral theorem¹

$$C_{\mathbf{k}} = \frac{i}{2\pi} \int \frac{d\omega}{e^{\omega/k_B T} + \eta} [g(\mathbf{k}, \omega + i0^+) - g(\mathbf{k}, \omega - i0^+)], \quad (7)$$

where T is the temperature and k_B is the Boltzmann constant.

In order to solve the equations of motion, the higher-order Green's functions appearing in Eq. (4) have to be decoupled. The following derivations make use of Fermionic Green's functions ($\eta = +1$) instead of the Bosonic Green's functions ($\eta = -1$) of earlier work, where zero eigenvalues of the equation of motion matrix have to be treated carefully, e.g.^{12,22}.

In previous work [12-19], the operators A and B were the spin operators:

$$A = S^\kappa, \kappa = +, -, z, \text{ and } B = (S^-)^m (S^z)^n, \quad (8)$$

where m and n are zero or positive integers, necessary for treating larger spin values S . The z -axis was chosen to be the particular direction in which the single-ion anisotropy is active.

In this paper, in order to treat the three directions in space on an equal footing, we use the following spin operators to construct the Green's functions:

$$A = S^\alpha, \alpha = x, y, z, \text{ and } B = (S^x)^l (S^y)^m (S^z)^n, \quad (9)$$

where l, m, n are integers or zero.

The advantage of such operators is that the S^α 's are equivalent to each other. A particular direction in space is not preferred.

Analogous to the usual formulation, we apply RPA to the terms coming from the exchange interaction in the new variables. This corresponds to the following factorization:

$$\langle\langle S_i^\alpha S_l^\beta; B_j \rangle\rangle = \langle S_i^\alpha \rangle \langle\langle S_l^\beta; B_j \rangle\rangle + \langle S_l^\beta \rangle \langle\langle S_i^\alpha; B_j \rangle\rangle, \alpha, \beta = x, y, z, \text{ and } i \neq l. \quad (10)$$

RPA is not an appropriate decoupling for the on-site terms coming from the single-ion anisotropy. For these, we use a generalization of the Anderson-Callen decoupling (originally derived only for the uniaxial out-of-plane anisotropies¹⁴) by assuming that the decoupling form factor Φ_α has an identical form in all spatial directions ($\alpha = x, y, z$).

$$\langle\langle S_i^\alpha S_i^\beta + S_i^\beta S_i^\alpha; B_j \rangle\rangle = \langle S_i^\alpha \rangle \Phi_\alpha \langle\langle S_i^\beta; B_j \rangle\rangle = \langle S_i^\beta \rangle \Phi_\beta \langle\langle S_i^\alpha; B_j \rangle\rangle, \alpha, \beta = x, y, z \text{ and } \alpha \neq \beta. \quad (11)$$

Here

$$\Phi_\alpha = 2 \left(1 - \frac{1}{2S^2} [S(S+1) - \langle S_i^\alpha S_i^\alpha \rangle] \right), \alpha = x, y, z. \quad (12)$$

As appropriate anti-commutator Green's functions we choose

$$\mathbf{G} = \begin{pmatrix} \langle\langle S_i^x; B_j \rangle\rangle_{+1} \\ \langle\langle S_i^y; B_j \rangle\rangle_{+1} \\ \langle\langle S_i^z; B_j \rangle\rangle_{+1} \end{pmatrix}. \quad (13)$$

Applying the decoupling procedures (10, 11), we obtain an equation of motion from which the Green's functions can be determined

$$(\omega \mathbf{I} - \mathbf{P}) \mathbf{g} = \mathbf{F}_{+1}^{ij} = \begin{pmatrix} \langle\langle [S_i^x; B_j]_{+1} \rangle\rangle \\ \langle\langle [S_i^y; B_j]_{+1} \rangle\rangle \\ \langle\langle [S_i^z; B_j]_{+1} \rangle\rangle \end{pmatrix}. \quad (14)$$

One of the main advantages of the present formulation is that the matrix \mathbf{P} turns out to be Hermitian, whereas in earlier work^{12,13,15,17}, the corresponding matrix at this stage of the decoupling was real and non-Hermitian.

$$\mathbf{P} = \begin{pmatrix} 0 & iH_z & -iH_y \\ -iH_z & 0 & iH_x \\ iH_y & -iH_x & 0 \end{pmatrix}. \quad (15)$$

Here

$$H_\alpha = \langle S^\alpha \rangle (J_0 - J_{\mathbf{k}}) + B_\alpha + K_{2\alpha} \langle S^\alpha \rangle \Phi_\alpha, \quad \alpha = x, y, z. \quad (16)$$

The quantities J 's are defined as

$$J_{\mathbf{k}} = J \sum_j e^{i\mathbf{k} \cdot \mathbf{a}_j} \text{ and } J_0 = \gamma J, \quad (17)$$

where the summation is over the nearest neighbours and γ is the number of nearest neighbours.

Because the matrix \mathbf{P} is Hermitian, it has real eigenvalues:

$$\omega_1 = 0, \omega_{2,3} = \pm \sqrt{H_x^2 + H_y^2 + H_z^2} = \pm E_{\mathbf{k}}. \quad (18)$$

The eigenvector matrix can be determined analytically, where the columns correspond to the eigenvalues $0, -E_{\mathbf{k}}, +E_{\mathbf{k}}$, respectively

$$\mathbf{U} = \begin{pmatrix} h_x/h_z & -(h_z - ih_x h_y)/(h_x + ih_y h_z) & -(h_z + ih_x h_y)/(h_x - ih_y h_z) \\ h_y/h_z & -i(h_x^2 + h_z^2)/(h_x + ih_y h_z) & i(h_x^2 + h_z^2)/(h_x - ih_y h_z) \\ 1 & 1 & 1 \end{pmatrix}, \quad (19)$$

and its inverse is

$$\mathbf{U}^{-1} = \frac{1}{2} \begin{pmatrix} 2h_x h_z & 2h_y h_z & 2h_z^2 \\ -h_x h_z - ih_y & -h_y h_z + ih_x & h_x^2 + h_y^2 \\ -h_x h_z + ih_y & -h_y h_z - ih_x & h_x^2 + h_y^2 \end{pmatrix}, \quad (20)$$

where we have defined

$$h_\alpha = \frac{H_\alpha}{E_{\mathbf{k}}}, \quad \alpha = x, y, z. \quad (21)$$

The Green's function is obtained by¹⁷

$$\mathbf{g}_{\mu\nu} = \sum_{\lambda=1}^3 \sum_{\tau=1}^3 \frac{U_{\mu\tau} U_{\tau\lambda}^{-1}}{\omega - \omega_\tau} F_{+1}^{\lambda\nu} = \sum_{\lambda=1}^3 \mathbf{R}_{\mu\lambda, \mathbf{k}} F_{+1}^{\lambda\nu}. \quad (22)$$

Applying the spectral theorem (7), we get the correlation functions (with $\eta = +1$) in momentum space

$$\mathbf{C}_{\mathbf{k}} = \begin{pmatrix} \langle BS^x \rangle \\ \langle BS^y \rangle \\ \langle BS^z \rangle \end{pmatrix} = \mathbf{R}_{\mathbf{k}} \mathbf{F}_{+1, \mathbf{k}}. \quad (23)$$

The index \mathbf{k} is introduced to indicate that the inhomogeneity for the anti-commutator is momentum-dependent, whereas that for the commutator is not.

Now we exploit the relation between the anti-commutator and commutator inhomogeneities,

$$\mathbf{F}_{+1, \mathbf{k}} = \mathbf{F}_{-1} + 2\mathbf{C}_{\mathbf{k}}, \quad (24)$$

to obtain

$$(\mathbf{I} - 2\mathbf{R}_{\mathbf{k}})\mathbf{C}_{\mathbf{k}} = \mathbf{R}_{\mathbf{k}}\mathbf{F}_{-1}. \quad (25)$$

This equation is written explicitly as follows

$$2 \begin{pmatrix} 0 & ih_z & -ih_y \\ -ih_z & 0 & ih_x \\ ih_y & -ih_x & 0 \end{pmatrix} \begin{pmatrix} C_{1\mathbf{k}} \\ C_{2\mathbf{k}} \\ C_{3\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \coth(E_{\mathbf{k}}/2k_B T) & -ih_z & ih_y \\ ih_z & \coth(E_{\mathbf{k}}/2k_B T) & -ih_x \\ -ih_y & ih_x & \coth(E_{\mathbf{k}}/2k_B T) \end{pmatrix} \begin{pmatrix} F_{-1,1} \\ F_{-1,2} \\ F_{-1,3} \end{pmatrix}. \quad (26)$$

It should be pointed out that these equations are not independent of each other: On the left hand side of equations (26), the first row multiplied by h_x plus the second row multiplied by h_y plus the third row multiplied by h_z is equal to zero. Applying the same condition to the right hand side, we find

$$h_x F_{-1,1} + h_y F_{-1,2} + h_z F_{-1,3} = 0. \quad (27)$$

Taking B of Eq. (9) as S^x , S^y and S^z , respectively, we get

$$h_y \langle S^z \rangle = h_z \langle S^y \rangle, \quad h_x \langle S^z \rangle = h_z \langle S^x \rangle \quad \text{and} \quad h_x \langle S^y \rangle = h_y \langle S^x \rangle. \quad (28)$$

Equations (27) and (28) are called regularity conditions because they are equivalent to similar equations in Ref.¹², which were derived there from the condition that the commutator Green's functions are regular at the origin, $\omega = 0$.

For the convenience of the discussion below, we now define two quantities Q_α and $h_{\alpha\beta}$ as

$$Q_\alpha = \frac{1}{N} \sum_{\mathbf{k}} \frac{\coth(E_{\mathbf{k}}/2k_B T)}{h_\alpha} \text{ and } h_{\alpha\beta} = \frac{h_\alpha}{h_\beta} = \frac{H_\alpha}{H_\beta}, \quad \alpha, \beta = x, y, z. \quad (29)$$

Before further discussion, we recall that Callen³ derived a general expression for calculating $\langle S^z \rangle$ only:

$$\langle S^z \rangle = \frac{(S - Q)(Q + 1)^{2S+1} + (S + 1 + Q)Q^{2S+1}}{(Q + 1)^{2S+1} - Q^{2S+1}}, \quad (30)$$

where S is the spin quantum number and $Q = \frac{1}{N} \sum_{\mathbf{k}} 1/(e^{\omega(\mathbf{k})/k_B T} - 1)$ with $\omega(\mathbf{k})$ being the dispersion relation. We found¹⁷ that putting Eq. (30) into a symmetric form has some formal advantage

$$\langle S^z \rangle = \frac{(2S + 1 - Q_1)(Q_1 + 1)^{2S+1} + (2S + 1 + Q_1)(Q_1 - 1)^{2S+1}}{2[(Q_1 + 1)^{2S+1} - (Q_1 - 1)^{2S+1}]}, \quad (31)$$

where $Q_1 = \frac{1}{N} \sum_{\mathbf{k}} \coth(\omega(\mathbf{k})/2k_B T) = 1 + 2Q$.

Now we are prepared to derive the required formulas for the components of the magnetization from Eqs. (26) and (27). We deal first with the case of an in-plane magnetization, say in the xy -plane. It is comparatively easy to get general expressions for this case. Then we proceed to the most general case, where it does not matter in which direction the magnetization points.

2.1. Magnetization in the xy -plane.

Here we take the magnetization to be in the xy -plane. In this case $\langle S^z \rangle = 0$ and $h_z = 0$, and we assume that $h_x \neq 0$, i.e. we select the x -direction as reference direction. Two of the Eqs. (26) can be rewritten as

$$\begin{aligned} -2C_3 &= iQ_x F_{-1,2} + F_{-1,3}, \\ -2h_{yx}C_1 + 2C_2 &= h_{yx}F_{-1,1} - F_{-1,2} + iQ_x F_{-1,3}. \end{aligned} \quad (32)$$

These equations allow us to obtain the expressions for the magnetization and all correlations for each spin value S by specifying the proper $B = (S^x)^l (S^y)^m (S^z)^n$ operators, and using the regularity conditions and some spin algebra. Because of the Anderson-Callen decoupling (11, 12), the correlations $\langle (S^x)^2 \rangle$, $\langle (S^y)^2 \rangle$ and $\langle (S^z)^2 \rangle$ are also needed. We list in Table I the explicit expressions for $\langle S^x \rangle$, $\langle (S^x)^2 \rangle$ and $\langle (S^y)^2 \rangle$ for spin quantum numbers $S = 1/2$ to $5/2$, where

$$P^2 = 1 + h_{yx}^2. \quad (33)$$

Note that this quantity is momentum independent due to the regularity conditions (28), $h_{yx} = \langle S^y \rangle / \langle S^x \rangle$.

Table I. The analytical expressions $\langle S^x \rangle$, $\langle (S^x)^2 \rangle$ and $\langle (S^y)^2 \rangle$ and for $S = 1/2$ to $5/2$.

S	$\langle S^x \rangle$	$\langle (S^x)^2 \rangle$	$\langle (S^y)^2 \rangle$
1/2	$1/2Q_x$	$1/4$	$1/4$
1	$\frac{4Q_x}{3Q_x^2 + P^2}$	$\frac{2(Q_x^2 + 1)}{3Q_x^2 + P^2}$	$\frac{2(Q_x^2 + h_{yx}^2)}{3Q_x^2 + P^2}$
3/2	$\frac{5Q_x^2 + P^2}{2Q_x(Q_x^2 + P^2)}$	$\frac{5Q_x^2 + 12 + P^2}{4(Q_x^2 + P^2)}$	$\frac{5Q_x^2 + R^2 + 12h_{yx}^2}{4(Q_x^2 + P^2)}$
2	$\frac{4Q_x(5Q_x^2 + 3P^2)}{5Q_x^4 + 10Q_x^2 P^2 + P^4}$	$\frac{10Q_x^4 + 42Q_x^2 + 6P^2 + 6Q_x^2 P^2}{5Q_x^4 + 10Q_x^2 P^2 + P^4}$	$\frac{10Q_x^4 + 42Q_x^2 h_{yx}^2 + 6P^2 h_{yx}^2 + 6Q_x^2 P^2}{5Q_x^4 + 10Q_x^2 P^2 + P^4}$
5/2	$\frac{35Q_x^4 + 42Q_x^2 P^2 + 3P^4}{2Q_x(3Q_x^4 + 10Q_x^2 P^2 + 3P^4)}$	$\frac{35Q_x^4 + 14Q_x^2(3P^2 + 16) + 3(P^2 + 32)P^2}{4(3Q_x^4 + 10Q_x^2 P^2 + 3P^4)}$	$\frac{35Q_x^4 + 14Q_x^2(3P^2 + 16h_{yx}^2) + 3(P^2 + 32h_{yx}^2)P^2}{4(3Q_x^4 + 10Q_x^2 P^2 + 3P^4)}$

For $P^2 = 1$ in the expression for $\langle S^x \rangle$ in Table I one obtains the same result as from Eq. (31) when substituting $S = 1/2$ to $5/2$ into it and replacing z by x .

With $P^2 = 1 + h_{yx}^2$, a general expression analogous to Eq. (31) is found

$$\langle S^x \rangle = \frac{[(2S + 1)P - Q_x](Q_x + P)^{2S+1} + [(2S + 1)P + Q_x](Q_x - P)^{2S+1}}{2P^2[(Q_x + P)^{2S+1} - (Q_x - P)^{2S+1}]}. \quad (34)$$

Substituting $S = 1/2$ to $5/2$ into Eq.(34), we obtain the expressions in the column 2 in Table I. Thus we suggest that Eq.(34) is the required correct expression for any S (we have no analytical proof for the general formula).

We also suggest the following analytical expressions for the three correlations for any spin value

$$\langle (S^x)^2 \rangle = \frac{2S(S+1) + Q_x S^x (P^2 - 3)}{2P^2}, \quad (35)$$

$$\langle (S^y)^2 \rangle = \frac{2S(S+1)h_{yx}^2 + (P^2 - 3h_{yx}^2)Q_x S^x}{2P^2}, \quad (36)$$

and

$$\langle (S^z)^2 \rangle = \frac{1}{2}Q_x S^x. \quad (37)$$

It is seen that the exact relation

$$\langle (S^x)^2 \rangle + \langle (S^y)^2 \rangle + \langle (S^z)^2 \rangle = S(S+1) \quad (38)$$

is satisfied. Also, when $S = 1/2$ to $5/2$ is substituted into Eqs.(35, 36), we obtain the expressions in columns 3 and 4 in Table I.

Because in the present case the x and y -directions should be equivalent, exchanging $x \longleftrightarrow y$ in Eqs.(34-37) and in Table I must also yield valid expressions.

2.2. The general case

We now take the z -direction as reference direction, supposing $h_z \neq 0$, and taking two equations from Eqs.(26)

$$\begin{aligned} 2C_2 - 2h_{yz}C_3 &= -iQ_z F_{-1,1} - F_{-1,2} + h_{yz}F_{-1,3}, \\ -2C_1 + h_{xz}C_3 &= F_{-1,1} - iQ_z F_{-1,2} - h_{xz}F_{-1,3}. \end{aligned} \quad (39)$$

Again, by specifying proper B operators, one obtains from these equations analytical expressions for the magnetization components and all correlations for each S . In Table II the explicit expressions for $\langle S^z \rangle$, $\langle (S^z)^2 \rangle$, $\langle (S^x)^2 \rangle$ and $\langle (S^y)^2 \rangle$ for spin quantum number $S = 1/2$ to $5/2$ are listed, where

$$R^2 = 1 + h_{xz}^2 + h_{yz}^2. \quad (40)$$

Table II. The analytical expressions for $\langle S^z \rangle$, $\langle (S^z)^2 \rangle$, $\langle (S^x)^2 \rangle$ and $\langle (S^y)^2 \rangle$ for $S = 1/2$ to $5/2$.

S	$\langle S^z \rangle$	$\langle (S^z)^2 \rangle$
1/2	$1/2 Q_z$	$1/4$
1	$\frac{4Q_z}{3Q_z^2 + R^2}$	$\frac{2(Q_z^2 + 1)}{3Q_z^2 + R^2}$
3/2	$\frac{5Q_z^3 + R^2}{2Q_z(Q_z^2 + R^2)}$	$\frac{5Q_z^2 + R^2 + 12}{4(Q_z^2 + R^2)}$
2	$\frac{4Q_z(5Q_z^3 + 3R^2)}{5Q_z^4 + 10Q_z^2 R^2 + R^4}$	$\frac{10Q_z^4 + 6Q_z^2(R^2 + 7) + 6R^2}{5Q_z^4 + 10Q_z^2 R^2 + R^4}$
5/2	$\frac{35Q_z^5 + 42Q_z^3 R^2 + 3R^4}{2Q_z(3Q_z^4 + 10Q_z^2 R^2 + 3R^4)}$	$\frac{35Q_z^4 + 14Q_z^2(3R^2 + 16) + 3(R^2 + 32)R^2}{4(3Q_z^4 + 10Q_z^2 R^2 + 3R^4)}$
S	$\langle (S^x)^2 \rangle$	$\langle (S^y)^2 \rangle$
1/2	$1/4$	$1/4$
1	$\frac{2(Q_z^2 + h_{yz}^2)}{3Q_z^2 + R^2}$	$\frac{2(Q_z^2 + h_{yz}^2)}{3Q_z^2 + R^2}$
3/2	$\frac{5Q_z^2 + R^2 + 12h_{xz}^2}{4(Q_z^2 + R^2)}$	$\frac{5Q_z^2 + R^2 + 12h_{yz}^2}{4(Q_z^2 + R^2)}$
2	$\frac{10Q_z^4 + 6Q_z^2(R^2 + 7h_{yz}^2) + 6R^2 h_{xz}^2}{5Q_z^4 + 10Q_z^2 R^2 + R^4}$	$\frac{10Q_z^4 + 6Q_z^2(R^2 + 7h_{xz}^2) + 6h_{yz}^2 R^2}{5Q_z^4 + 10Q_z^2 R^2 + R^4}$
5/2	$\frac{35Q_z^4 + 14Q_z^2(3R^2 + 16h_{yz}^2) + 3(R^2 + 32h_{xz}^2)R^2}{4(3Q_z^4 + 10Q_z^2 R^2 + 3R^4)}$	$\frac{35Q_z^4 + 14Q_z^2(3R^2 + 16h_{xz}^2) + 3(R^2 + 32h_{yz}^2)R^2}{4(3Q_z^4 + 10Q_z^2 R^2 + 3R^4)}$

Similar to the case in subsection 2.1, we suggest that these quantities can be expressed by the following equations for any S .

$$\langle S^z \rangle = \frac{[(2S+1)R - Q_z](Q_z + R)^{2S+1} + [(2S+1)R + Q_z](Q_z - R)^{2S+1}}{2R^2[(Q_z + R)^{2S+1} - (Q_z - R)^{2S+1}]}, \quad (41)$$

$$\langle (S^z)^2 \rangle = \frac{2S(S+1) + (R^2 - 3)Q_z S^z}{2R^2}, \quad (42)$$

$$\langle (S^x)^2 \rangle = \frac{2S(S+1)h_{xz}^2 + (R^2 - 3h_{xz}^2)Q_z S^z}{2R^2}, \quad (43)$$

and

$$\langle (S^y)^2 \rangle = \frac{2S(S+1)h_{yz}^2 + (R^2 - 3h_{yz}^2)Q_z S^z}{2R^2}. \quad (44)$$

Here equation (38) is again satisfied. As long as $\langle S^z \rangle$ is calculated, the other two components of the magnetization can be computed from the regularity conditions Eqs.(28).

Because none of the three directions is special, we can also pick the x - or y -direction as reference direction. Therefore, in Eqs. (41-44) and in Table II, the formulas remain valid when performing the exchanges of coordinates, e.g., $x \rightarrow z \rightarrow y \rightarrow x$. Note too, that the expressions of Eqs. (41-44) revert to those of Eqs. (34-37) of subsection 2.1 after making the exchange $x \rightarrow y \rightarrow z \rightarrow x$ and setting $h_{zx} = 0$.

2.3. The effective (temperature-dependent) anisotropies

The absolute value of the magnetization and the equilibrium angles θ_0 and φ_0 of the magnetization direction are determined by the following equations:

$$M^2(T) = \langle S^x \rangle^2 + \langle S^y \rangle^2 + \langle S^z \rangle^2, \quad (45)$$

$$\theta_0 = \arctan \frac{\sqrt{\langle S^x \rangle^2 + \langle S^y \rangle^2}}{\langle S^z \rangle}, \quad \varphi_0 = \arctan \frac{\langle S^y \rangle}{\langle S^x \rangle}. \quad (46)$$

Fröbrich et al.¹² have determined the effective (temperature-dependent) anisotropy coefficients $K_{2z}(T)$ non-perturbatively for the out-of-plane anisotropy case by minimizing the free energy with respect to the orientation angles of the magnetization. In this paper, we are also able to determine the coefficients $K_{2x}(T)$ and $K_{2y}(T)$ in the same manner.

The free energy corresponding to the Heisenberg model with anisotropies in each direction reads

$$\begin{aligned} F(T) = & F_0(T) - K_{2x}(T) \sin^2 \theta \cos^2 \varphi - K_{2y}(T) \sin^2 \theta \sin^2 \varphi - K_{2z}(T) \cos^2 \theta \\ & - B_x M \sin \theta \cos \varphi - B_y M \sin \theta \sin \varphi - B_z M \cos \theta \end{aligned} \quad (47)$$

We have mentioned that, due to the relation $(S^x)^2 + (S^y)^2 + (S^z)^2 = S(S+1)$, the three anisotropies are not independent of each other. Therefore we are allowed to transform for instance $K_{2x} \rightarrow K_{2x} - K_{2y}$, $K_{2y} \rightarrow 0$, and $K_{2z} \rightarrow K_{2z} - K_{2y}$.

Choosing the xz -plane as reorientation plane by taking $B_y = 0$, which leads to $\varphi = 0$, the variation of $dF/d\theta = 0$ yields

$$K_{2z}(T) - K_{2x}(T) = \frac{B_x M \cos \theta_0 - B_z M \sin \theta_0}{2 \sin \theta_0 \cos \theta_0}. \quad (48)$$

The result of the uniaxial out-of plane case¹² is obtained by taking $K_{2x} = 0$. The angle θ_0 is the equilibrium angle.

When considering for example the in-plane magnetization with $K_{2x} \neq 0$ and $K_{2y} \neq 0$ and $K_{2z} = 0$ (no out-of-plane anisotropy), one has two equations,

$$dF(T)/d\theta = 0, \quad (49)$$

and

$$dF(T)/d\varphi = 0 \quad (50)$$

to determine $K_{2x}(T)$ and $K_{2y}(T)$ with the result:

$$\begin{aligned} K_{2x}(T) &= \frac{B_z M}{2 \cos \theta_0} - \frac{B_x M}{2 \sin \theta_0 \cos \varphi_0}, \\ K_{2y}(T) &= \frac{B_z M}{2 \cos \theta_0} - \frac{B_y M}{2 \sin \theta_0 \sin \varphi_0}, \end{aligned} \quad (51)$$

where the angles θ_0, φ_0 are to be considered as equilibrium angles.

III. NUMERICAL RESULTS

In the numerical calculations, the strength of the exchange energy is set to $J = 100$. The parameters are scaled as in Refs.^{12,13},

$$J \rightarrow J/S(S+1), \quad B \rightarrow B/S, \quad K_2 \rightarrow K_2/S(S-1/2). \quad (52)$$

Scaling is introduced to obtain magnetization curves which are approximately universal for different spin values S . The scaling of K_2 guarantees the property $\lim_{T \rightarrow 0} K_2(T)/K_2 = 1$. For the 3-dimensional (3D) case, we use a simple cubic lattice and for the 2-dimensional (2D) case, a square lattice.

3.1. The 3D case

For the 3D examples, we always put $K_{2z} = 0$ and $K_{2x} = 1$. For the uniaxial in-plane case ($K_{2y} = 0$) the magnetization points in the x -direction. In the absence of magnetic fields, the corresponding scaled Curie point $T_c/T_c(S=1)$, normalized to that of $S=1$, versus the spin quantum number S is plotted as squares in Fig.1. The scaled T_c slightly decreases with increasing S .

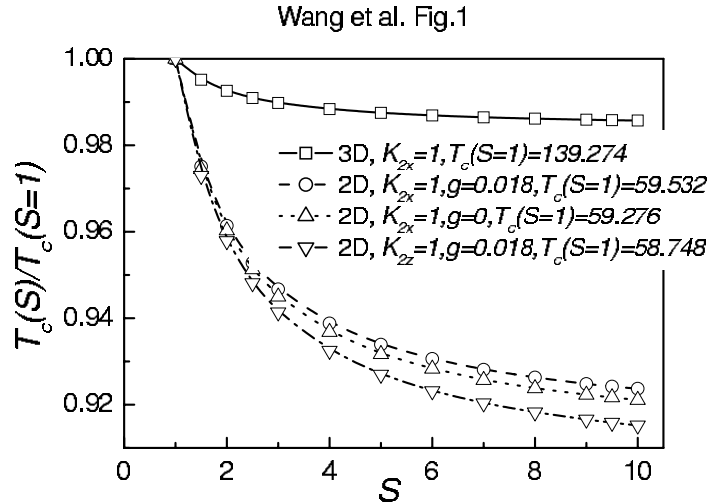


FIG. 1: The scaled Curie temperature T_c versus the spin quantum number S when there is only a single-ion anisotropy in one direction. Squares: 3D case. Upward triangles: 2D case without dipole-dipole interaction. Circles and downward triangles : 2D case with dipole-dipole interaction (with strength $g = 0.018$), when the easy-axis is in plane and out of plane, respectively.

We show some examples when including a magnetic field $\mathbf{B} = (B_x, B_y, B_z)$ in addition to the anisotropies $K_{2x} = 1, K_{2y} \neq 0, K_{2z} = 0$. The direction of the magnetization will ultimately turn towards the field direction when

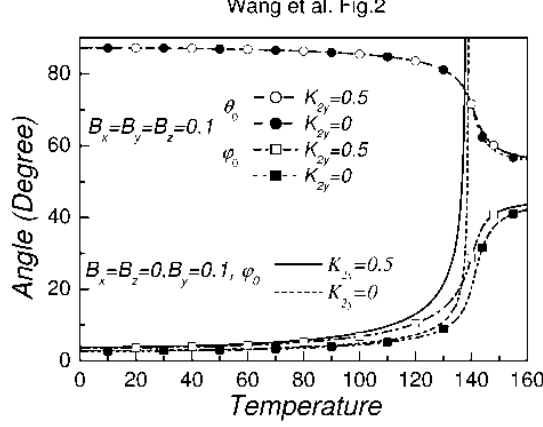


FIG. 2: The angles of the direction of the magnetization (θ_0 , φ_0), defined by Eqs.(46), as functions of the temperature for $K_{2z} = 0$, $K_{2x} = 1$ and various K_{2y} anisotropies and magnetic fields. The symbols are just to label curves.

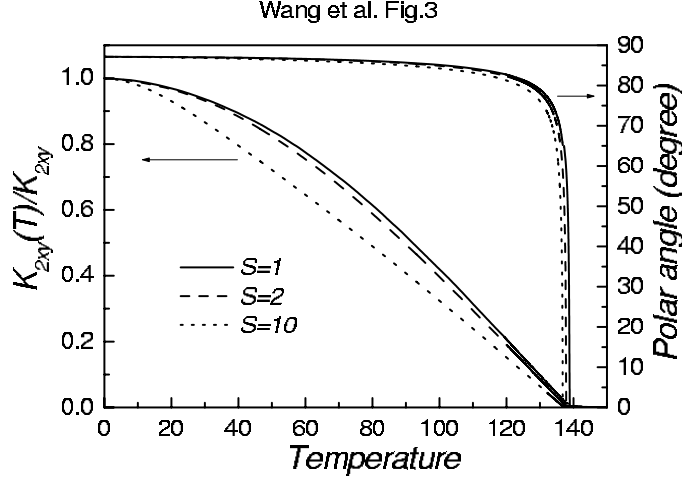


FIG. 3: The effective anisotropy $K_{2xy}(T)/K_{2xy}(T=0)$ and the equilibrium polar angle θ_0 for $S = 1, 2$ and 10 in the 3D case for in-plane anisotropy. The parameters are $K_{2xy} = K_{2x} = K_{2y} = 1$ and $B_z = 0.1$.

the temperature goes above the Curie point (defined from $\langle S^x \rangle = 0$ for the field-free case). For instance, when $\mathbf{B} = (0.1, 0.1, 0.1)$, (θ_0, φ_0) approach $(57.74, 45)$ degrees, which is the $[111]$ direction, and when $\mathbf{B} = (0, 0.1, 0)$, φ_0 approaches 90 degrees, as shown in Fig. 2. However, at low temperature, where the field is not strong enough to overcome the effect of the anisotropy, the magnetization will be close to the direction along which the anisotropy is strongest. With increasing temperature, the magnetization gradually turns towards the field direction. At zero temperature, the initial angles of φ_0 are 3.60 and 2.74 degrees for $K_{2y} = 0.5$ and 0, respectively, for both applied fields $\mathbf{B} = (0.1, 0.1, 0.1)$ and $(0, 0.1, 0)$. When $K_{2y} = 0.5$, the magnetization turns more easily than with $K_{2y} = 0$. Note that the dashed and dot-dashed lines are very similar. This reflects the fact that the magnetization component in the plane is almost the same for the two cases of $K_{2y} = 0.5$ and 0. If $\mathbf{B} = (0.1, 0.1, 0)$, the magnetization is in the

Wang et al. Fig.4

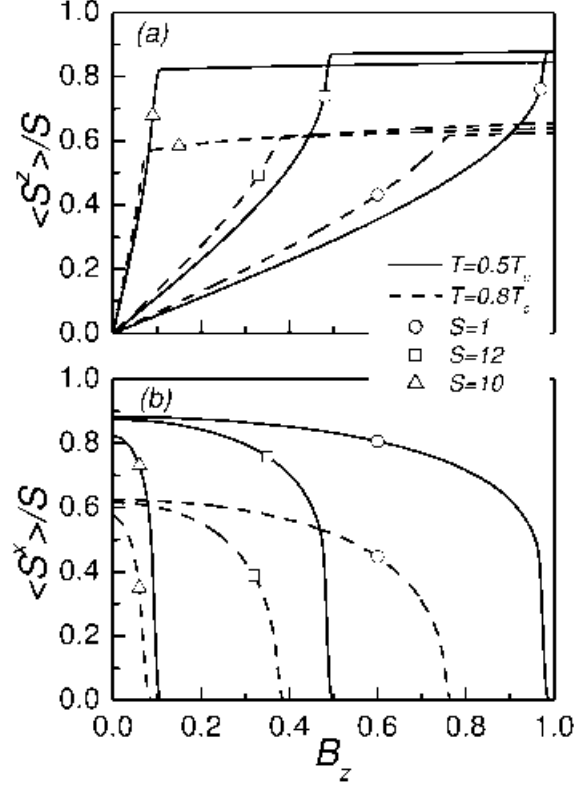


FIG. 4: The components of the magnetization (a) $\langle S^z \rangle / S$ and (b) $\langle S^x \rangle / S$ as functions of the external field in z -direction B_z for $S = 1, 2$ and 10 and at temperatures $T = 0.5T_c$ and $0.8T_c$. T_c is the scaled Curie temperature of the 3D case shown by squares in Fig.1.

xy -plane ($\theta_0 = 90^\circ$). The curve of the angle φ_0 versus temperature is identical to the solid line in Fig. 2 for $K_{2y} = 0.5$ and to the dotted line for $K_{2y} = 0$.

As a further example we discuss the in-plane anisotropy case, with $K_{2xy} = K_{2x} = K_{2y} = 1$. The effective anisotropy coefficient as a function of the temperature can be calculated by Eq. (51). Figure 3 shows examples for the spin values $S = 1, 2$ and 10 calculated for $B_z = 0.1$ and $B_x = B_y = 0$. At zero temperature, $K_{2xy}(T = 0)$ is the same as the anisotropy parameter of the Hamiltonian K_{2xy} . With increasing temperature, $K_{2xy}(T)$ decreases. Close to the Curie point, the coefficients approach zero. With the present choice of parameters the reorientation temperature is close to the Curie point; in general they can be quite different. In the intermediate temperature range, one observes a sensitivity to the spin value: the larger the spin S , the smaller the effective coefficient. The larger the spin the more increases the range of a linear behaviour of the effective anisotropy, which is in accordance with mean field results

where for $S \rightarrow \infty$ or for classical spins one obtains a linear behaviour $K_2(T) = K_2(0)(1 - T/T_C)^{23}$. Figure 3 also shows the corresponding equilibrium angle θ_0 defined by Eq.(46). The in-plane anisotropy should force the magnetization into the xy -plane. However, because of a small field in z -direction $B_z = 0.1$, the magnetization deviates slightly from the plane at zero temperature, and there is a small initial angle. It is the same for each S . With increasing temperature, the magnetization reorients slowly, owing to the action of the field. Close to the Curie point, the effective anisotropy approaches zero, so that the magnetization reorients rapidly in the direction of the z -axis, the direction of the external field.

The orientation angle θ_0 of the magnetization depends on the temperature as well as on the external field. In Figure 4, we plot the magnetization components $\langle S^x \rangle / S$ and $\langle S^z \rangle / S$ versus the unscaled external field B_z at two temperatures for $S = 1, 2$ and 10 . Because of scaling the temperature dependence for different spin values looks similar. The reorientation fields at which the reorientation to the field direction has occurred however are different and are given by $B_z = 0.76, 0.38$ and 0.08 , respectively at $T = 0.8T_C$. The larger the spin value S , the easier is the reorientation of the magnetization. To compare the reorientation behaviour at different temperatures, we also show the results at $T = 0.5T_C$. In this case, the magnitudes of the field at which the magnetization reorientation occurs are $B_z = 0.98, 0.49$ and 0.10 , respectively, which are higher than those at temperature $T = 0.8T_C$. At a lower temperature, it is more difficult for the magnetization to turn under the action of the field, as one expects.

3.2. The 2D-case (monolayer)

For the discussion of a monolayer (the 2D-case), we add the dipole-dipole interaction (DI) to the Hamiltonian of Eq.(1)

$$\begin{aligned} & \frac{g}{2} \sum_{ij} \frac{\mathbf{S}_i \cdot \mathbf{S}_j - 3(\mathbf{S}_i \cdot \mathbf{u}_{ij})(\mathbf{S}_j \cdot \mathbf{u}_{ij})}{r_{ij}^3} \\ &= \sum_{ij} \frac{g}{2r_{ij}^3} \{S_i^x S_j^x [1 - 3(u_{ij}^x)^2] + S_i^y S_j^y [1 - 3(u_{ij}^y)^2] + S_i^z S_j^z [1 - 3(u_{ij}^z)^2]\}, \end{aligned} \quad (53)$$

where r_{ij} is the distance between sites i and j , and its components along three axes are $r_{ij}u_{ij}^x$, $r_{ij}u_{ij}^y$ and $r_{ij}u_{ij}^z$, respectively. The higher-order Green's functions containing DI terms are also decoupled by RPA, i.e. by Eq.(10). As a result, there appear additive terms due to DI in H_α of Eq.(16), which include non-dispersive parts as well as dispersive parts. As an approximation, we neglect the dispersive parts and retain the non-dispersive parts only. Such an approximation was used before in Ref.¹³. The full RPA treatment of the dipole coupling would require complex arithmetic numerically (see Appendix A of Ref.¹³). An exception is the uniaxial out-of-plane case, for which it was shown in this Appendix that the mean-field results are close to RPA. Using complex arithmetic numerically is not in principle a hindrance, but is quite tedious to perform. One obtains

$$H_\alpha = \langle S^\alpha \rangle (J_0 - J_{\mathbf{k}}) + B_\alpha + K_{2\alpha} \langle S^\alpha \rangle \Phi_\alpha - g \langle S^\alpha \rangle \sum_l \frac{1}{r_{0l}^3} [1 - 3 \frac{(u_{0l}^\alpha)^2}{r_{0l}^2}], \quad \alpha = x, y, z. \quad (54)$$

In the last term of Eq.(54), the subscript 0 means the origin, and the summation covers all lattice sites except for the origin. The lattice sum can be done and Eq.(54) becomes explicitly

$$\begin{aligned} H_{x,y} &= \langle S^{x,y} \rangle (J_0 - J_{\mathbf{k}}) + B_{x,y} + K_{2x,y} \langle S^{x,y} \rangle \Phi_{x,y} + gT_0 \langle S^{x,y} \rangle, \\ H_z &= \langle S^z \rangle (J_0 - J_{\mathbf{k}}) + B_z + K_{2z} \langle S^z \rangle \Phi_z - 2gT_0 \langle S^z \rangle, \end{aligned} \quad (55)$$

where $T_0 = \sum_{l,m} \frac{l^2}{(l^2 + m^2)^{5/2}} = 4.5165$. To compare with the results in Ref.¹³, we choose $g = 0.018$ (a value which corresponds to Ni with the present set of parameters) in most cases. Note that the DI strength g is also scaled as

$$g \rightarrow g/S(S+1). \quad (56)$$

Correspondingly, the expressions for the effective anisotropies Eqs.(48, 51) will have additional terms coming from the DI, as in Ref.¹³ for the out-of-plane case.

Now we proceed to some numerical examples. Owing to the Mermin-Wagner theorem²⁴, a Heisenberg monolayer without some kind of anisotropy has no spontaneous magnetization. A spontaneous magnetization can be achieved by DI alone. Figure 5 shows the absolute value of the in-plane magnetization due to the action of DI as function of

the temperature. One observes that for different spin quantum numbers S , the scaled Curie temperature T_c is the same for a fixed DI strength. The inner panel shows the $T_c - g$ curve in the range of $g = 0.01 - 1$. When g approaches zero, T_c decreases drastically, and approaches zero for $g \rightarrow 0$ in accordance with the Mermin-Wagner theorem.

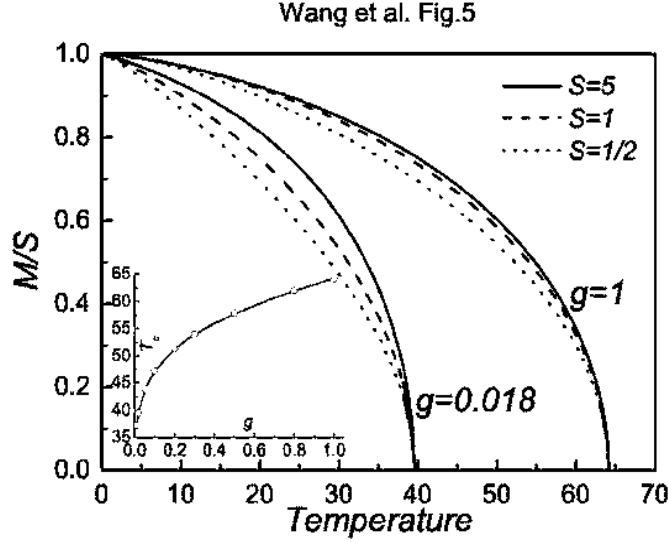


FIG. 5: Magnetization-temperature curve for $S = 1, 2$ and 5 for the monolayer with DI strength $g = 0.018$ and 1 , respectively. M is the magnetization defined in Eq.(45) for the in-plane situation. When g is fixed, T_c is same for any S . The inner panel: T_c as a function of the DI strength g .

If there is only a single-ion anisotropy in addition to the Heisenberg exchange energy term, a spontaneous magnetization of the monolayer is also induced. The upward triangles in Fig.1 show the scaled Curie temperature T_c as a function of S when there is an in-plane anisotropy in one direction. The Curie temperatures are lower and decrease more rapidly than those for the 3D case. The Curie points for the 2D case are lower than those for the 3D case for the same S , since the number of nearest neighbours of each site in a 2D square lattice is four, while that in a cubic 3D lattice is six.

With an external field in addition to the single-ion anisotropies, the magnetization will rotate. The rotation in the monolayer case exhibits (except for the temperature scale) the same features as those of the 3D system. If we plot the $\theta_0, \varphi_0 - T$ curves, the qualitative behaviour will be the same as in Fig.2. With the same parameters, the initial angles are the same as in Fig.2. If, for example, $\mathbf{B} = (0.1, 0.1, 0.1)$, $K_{2z} = 0$ and $K_{2x} = 1$, the angles (θ_0, φ_0) at zero temperature are $(87.26, 3.61)$ degrees for $K_{2y} = 0.5$ and $(87.26, 2.64)$ degrees for $K_{2y} = 0$. Above the Curie point, (θ_0, φ_0) again approach the field direction $(57.74, 45)$ degrees, i.e. the $[111]$ direction.

Including both the single-ion anisotropy and DI, we plot in Fig. 1 the scaled Curie temperature T_c as a function of S for the uniaxial cases $K_{2x} = 1$ (in-plane) and $K_{2z} = 1$ (out-of-plane) using $g = 0.018$. It is seen that, if the easy-axis is along the out-of-plane direction, the effect of DI is to lower T_c . If the easy-axis is in the in-plane direction, the effect of DI is to raise T_c . This is clear from Eqs.(55) where the effect of DI can be understood as a renormalization of the non-dispersive exchange interaction terms:

$$\begin{aligned} J_0 \langle S^{x,y} \rangle &\rightarrow (J_0 + gT_0) \langle S^{x,y} \rangle, \\ J_0 \langle S^z \rangle &\rightarrow (J_0 - 2gT_0) \langle S^z \rangle. \end{aligned} \quad (57)$$

$J_{\mathbf{k}}$ in Eq.(55) is kept unchanged. As a result, the exchange energy strength along the z -direction is suppressed and that in the xy -plane is enhanced. The figure shows that in the out-of-plane case, the Curie temperature T_c decreases (compared to $g = 0$) more strongly than it increases for the in-plane case.

Now we investigate the in-plane (or easy-plane) anisotropy case, where $K_{2xy} = K_{2x} = K_{2y} = 1$. Figure 6 shows the effective anisotropy coefficient, defined by Eq.(51), as a function of the temperature for $S = 1, 2$ and 10 , when $B_z = 0.1$ is taken. At zero temperature, $K_{2xy}(0)$ is the same as the parameter K_{2xy} . The effective anisotropy decreases with increasing temperature, and at the Curie point it approaches zero. In the intermediate temperature range it is

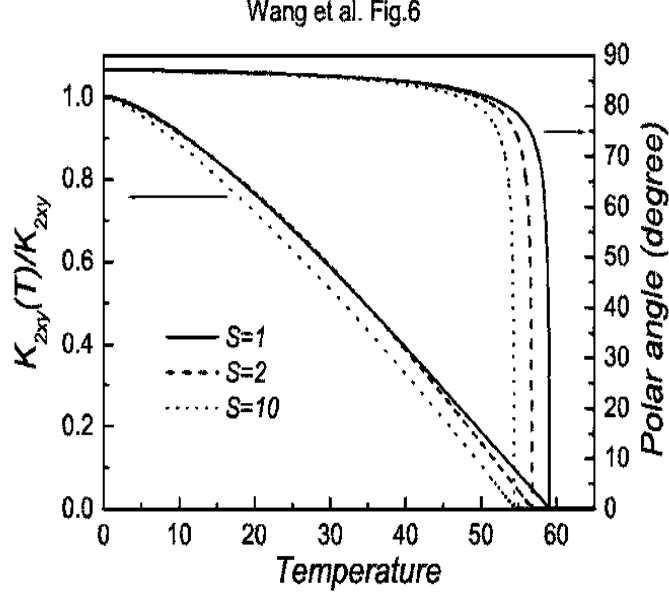


FIG. 6: Effective anisotropy $K_{2xy}(T)/K_{2xy}$ and equilibrium polar angle θ_0 for $S = 1, 2$ and 10 in the 2D case. The parameters are same as in Fig. 3.

the smaller the larger the spin quantum number S is. Figure 6 also shows the equilibrium polar angle θ_0 defined by Eq.(46) when $B_z = 0.1$. All the properties in Fig.6 are similar to those in Fig.3. The only difference is that the Curie temperatures in the 2D case are by more than a factor of two smaller (Fig.1) and more different for the various spin values (Fig.6) than in the 3D case (Fig.3).

The polar angle of the magnetization depends on the temperature as well as on the external field. It is unnecessary to plot the components of the magnetization as functions of the external field at various temperatures as in Fig. 4 (the 3D case) because they are qualitatively so similar.

In Refs.^{12,13}, the case of the out-of-plane anisotropy was studied in detail. Since the method developed in the present paper also enables the study of the in-plane anisotropy, it is natural to compare both cases. We mention the following differences, which can all be explained on the basis of Eqs. (55). The first concerns the case where there is no external field. For an out-of-plane anisotropy, there is a magnetization reorientation from the z -direction to the xy -plane due to DI even without an external field¹³. At zero temperature, the magnetization points to the z -direction because of the out-of-plane anisotropy term K_{2z} . With increasing temperature, the magnetization turns to the xy -plane owing to the DI. In the case of in-plane anisotropy, there is no spin reorientation in the absence of the field, because the magnetization is already in the xy -plane at zero temperature.

Secondly, with the same DI strength and the same field (perpendicular to the anisotropy direction), the magnetization reorientation temperature is different for the two anisotropy cases as shown in Figure 7. In Fig.7(a) and (b), the solid lines are for $S = 1$ and the dotted lines are for $S = 10$, both with $g = 0.018$. Figure 7(a) depicts the in-plane anisotropy case with an external field $B_z = 0.1$ along the z -direction, and figure 7(b) the out-of-plane anisotropy case with an external field $B_x = 0.1$ along the x -direction. The magnetization reorientation temperature of the latter case is lower than that of the former case. This can be understood from Eqs. (55), from which one sees that the dipole interaction enhances the effect of the in-plane anisotropy term, whereas the opposite is true for the out-of-plane case; i.e. the role of DI can be considered as a renormalization of the anisotropy terms in the following sense

$$\begin{aligned} K_{2x,y}\Phi_{x,y} &\rightarrow K_{2x,y}\Phi_{x,y} + gT_0, \\ K_{2z}\Phi_z &\rightarrow K_{2z}\Phi_z - 2gT_0. \end{aligned} \quad (58)$$

This also explains, thirdly, the effect of the variation in the strength of the DI, as shown in Figure 7(a) and (b). In the case of in-plane anisotropy, increasing the DI strength hinders the reorientation from in-plane to out-of-plane, see Fig.7(a), whereas the reorientation from out-of-plane to in-plane is enforced in the case of the out-of-plane anisotropy. It is seen that the DI suppresses the out-of-plane anisotropy and enhances the in-plane anisotropy.

Wang et al. Fig.7

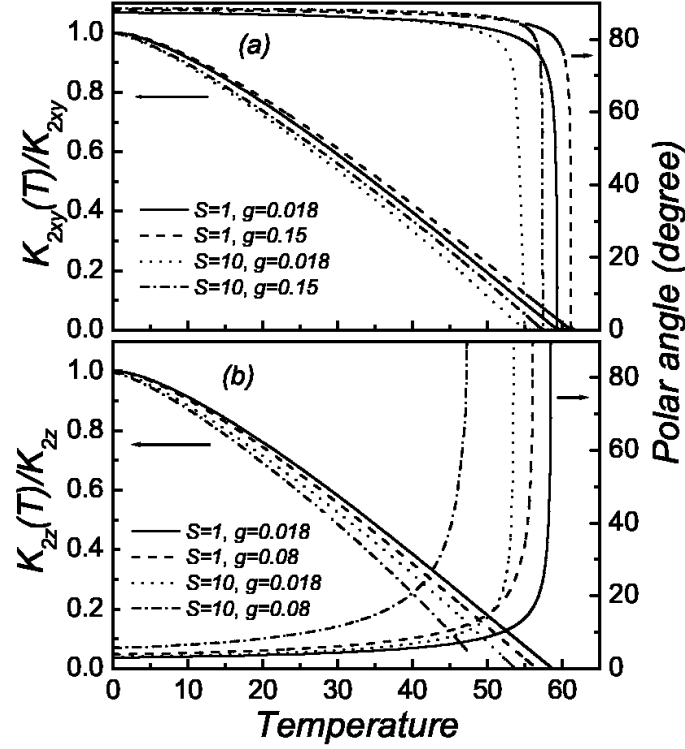


FIG. 7: (a) Effective anisotropy $K_{2xy}(T)/K_{2xy}$ and equilibrium polar angle θ_0 for $S = 1$ and 10 for the monolayer with DI strengths $g = 0.018$ and 0.15 for the in-plane case. The parameters are $K_{2xy} = 1$ and $B_z = 0.1$. (b) Effective anisotropy $K_{2z}(T)/K_{2z}$ and equilibrium polar angle θ_0 for $S = 1$ and 10 for the monolayer with DI strengths $g = 0.018$ and 0.08 for the out-of-plane case. The parameters are $K_{2z} = 1$ and $B_x = 0.1$.

The fourth difference involves the variation of the external field. If an external field B_x is applied along the x -direction in the case of an out-of-plane anisotropy, the magnetization reorients easier with DI than without DI. This is shown by comparison of the dashed and solid lines in Fig.8. The reason is that we can also interpret the effect of the DI as a renormalization of the external field, as has been done in Ref.¹³, see Eq. (55)

$$\begin{aligned} B_{x,y} &\rightarrow B_{x,y} + gT_0\langle S^{x,y} \rangle, \\ B_z &\rightarrow B_z - 2gT_0\langle S^z \rangle. \end{aligned} \quad (59)$$

This means that the effect of the DI is to enhance a magnetic field in the xy -plane, and to weaken an external field along the z -direction. Therefore, if an external field B_z is applied along the z -direction in the case of an in-plane anisotropy, it is more difficult for the magnetization to reorient into the out-of-plane direction with DI than without DI. Comparison of the dotted and solid lines in Fig.8 provides an example.

IV. CONCLUSIONS AND DISCUSSION

In this paper, we have treated a Heisenberg Hamiltonian with single-ion anisotropies in all three directions of space by applying many-body Green's function theory, thus generalizing previous work dealing with uniaxial out-of-plane anisotropy. To do so, we selected the spin operators S^x , S^y and S^z as basis operators to construct the Green's functions instead of the commonly used operators S^+ , S^- and S^z . We stress that in the derivation of the formalism none of the three axes is special, so that we are always able to select a reference direction along which the magnetization

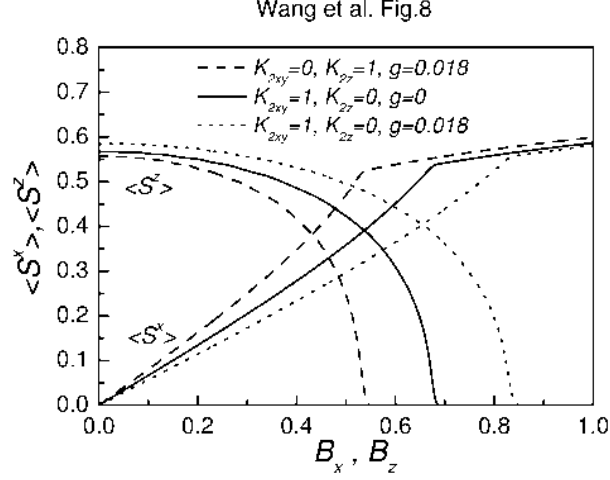


FIG. 8: The components of the magnetization $\langle S^x \rangle$ and $\langle S^z \rangle$ as functions of the external field for $S = 1$ at the temperature $T/T_c = 0.8$. The dashed lines correspond to the out-of-plane anisotropy with a field B_x in x -direction. The solid and dotted lines correspond to the in-plane anisotropy with a field B_z in z -direction. If $K_{2xy} = 0$, $K_{2z} = 1$ and $g = 0$ and a field B_x , the corresponding magnetization curves are identical to the solid lines with $\langle S^x \rangle$ and $\langle S^z \rangle$ exchanged.

component is not zero. The key is the generalization of the Anderson-Callen decoupling to the terms from the single-ion anisotropy in all directions of space, Eqs.(11, 12). A formal advantage of the use of the present operators is that the matrix governing the equations of motion is Hermitian, whereas the usual formalism leads to real non-Hermitian matrices, which are more difficult to treat. A main result of the paper is that analytical expressions can be derived for the three components of the magnetization and the correlations $\langle (S^x)^2 \rangle$, $\langle (S^y)^2 \rangle$ and $\langle (S^z)^2 \rangle$ for any spin quantum number. The formalism obtained in this paper enables a treatment of both the in-plane and out-of-plane anisotropies.

Numerical calculations were carried out for various parameters for both 3D and 2D systems.

For the 2D system, we included the dipole-dipole interaction. Its effect on the magnetization can be explained on the basis of Eq.(55), and can be interpreted as a renormalization of the nondispersive part of the exchange interaction terms, or of the single-ion anisotropy terms or of the external field, see Eqs.(57, 58, 59). The reorientation of the magnetization from in-plane to out-of-plane under an external field occurs more easily without the DI than with it, or in other words the DI supports the reorientation from the out-of plane to the in-plane direction.

Because of Eq.(55), H_z may appear negative. In this case the regularity condition Eq.(28) would be meaningless because the z -component magnetization should be within $0 < \langle S^z \rangle < S$. Only when the value of g is under a certain value can there is a non-zero $\langle S^z \rangle$ without a field in z -direction. From Eq.(58), the condition should be $gT_0 < S(K_{2z}\Phi_z - 2gT_0)$. Then one should have $2SK_{2z}(1 - \frac{1}{2S^2}[S(S+1) - \langle S^z S^z \rangle]) > gT_0(1 + 2S)$. Since $\langle S^z S^z \rangle \geq S(S+1)/3$, one has $g < 2K_{2z}(2S-1)/3T_0(1+2S) = 0.1476(2S-1)/(1+2S)$, where $K_{2z} = 1$ is taken. The upper limit increases with spin quantum number. However, because we use scaled parameters in this paper, Eq.(52), we have $g < S(S+1)2K_{2z}(2S-1)/3T_0(1+2S)S(S-1/2) = (S+1)4/3T_0(1+2S) = 0.2952(S+1)/(2S+1)$. The upper limit decreases with spin quantum number. When the value of g is over this limit, the z -component of magnetization has to be zero. Figure 5 provides an example where the magnetization lies in the plane.

Finally, we point out that the numerical results are all calculated with scaled parameters in order to obtain universal results, in accordance with Refs.^{12,13}. With increasing S , the scaled exchange J and anisotropy K_2 become smaller as can be seen in Eq.(52). This results in the conclusions in Section 3 that, with increasing S , the following quantities decrease: the scaled T_c in Fig.1, the effective anisotropy coefficients in Figs.3, 6 and 7, and the field under which the reorientation occurs in Fig.4. If the parameters are not scaled but kept unchanged, the conclusions are the other way round. A larger S means a larger magnetization. It will, therefore, result in a higher Curie temperature. Consequently, the effective anisotropy coefficients are larger for larger S at a given temperature. For instance, at zero temperature, the effective anisotropy coefficient should be $K_2S(S-1/2)$. A larger magnetization is more difficult to turn by an external field. As a result, the magnitude of the field at which the magnetization reorientation occurs should rise with increasing S for a given temperature.

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